Thiophene, tetrabromo-

Other names:	2,3,4,5-tetrabromothiophene perbromothiophene tetrabromothiophene
Inchi:	InChI=1S/C4Br4S/c5-1-2(6)4(8)9-3(1)7
InchiKey:	AVPWUAFYDNQGNZ-UHFFFAOYSA-N
Formula:	C4Br4S
SMILES:	Brc1sc(Br)c(Br)c1Br
Mol. weight [g/mol]:	399.72
CAS:	3958-03-0

Physical Properties

Property code	Value	Unit	Source
ie	8.53	eV	NIST Webbook
log10ws	-5.88		Crippen Method
logp	4.798		Crippen Method
mcvol	134.110	ml/mol	McGowan Method
tb	599.20	K	NIST Webbook
tf	391.75	K	Solubility and solution thermodynamics of 2,3,4,5-tetrabromothiophene in (ethanol + trichloromethane) binary solvent mixtures

Sources

Measurement and correlation of the solubility of 2,3,4,5-tetrabromothiophene in different solvents:	https://www.doi.org/10.1016/j.jct.2012.06.005
Solubility and solution thermodynamics of 2,3,4,5-tetrabromothiophene in (ethanol + tetrahydrofuran) binary solvent mixtures:	https://www.doi.org/10.1016/j.jct.2013.05.023
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3958030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility and solution thermodynamics of 2,3,4,5-tetrabromothiophene in (ethanol + trichloromethane) binary solvent mixtures:	https://www.doi.org/10.1016/j.fluid.2013.11.023

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point